

New representation of orbital motion with arbitrary angular momenta

Y. Suzuki¹, J. Usukura², and K. Varga^{1,3}

¹*Department of Physics, Faculty of Science, Niigata University, Niigata 950-21, Japan*

²*Graduate School of Science and Technology, Niigata University, Niigata 950-21, Japan*

³*Institute of Nuclear Research of the Hungarian Academy of Sciences, Debrecen, H-4001, Hungary*

(February 9, 2008)

Abstract

A new formulation is presented for a variational calculation of N -body systems on a correlated Gaussian basis with arbitrary angular momenta. The rotational motion of the system is described with a single spherical harmonic of the total angular momentum L , and thereby needs no explicit coupling of partial waves between particles. A simple generating function for the correlated Gaussian is exploited to derive the matrix elements. The formulation is applied to various Coulomb three-body systems such as $e^-e^-e^+$, $tt\mu$, $td\mu$, and αe^-e^- up to $L = 4$ in order to show its usefulness and versatility. A stochastic selection of the basis functions yields good results for various angular momentum states.

PACS numbers: 31.15.Pf, 31.25.-v, 36.10.-k, 02.60.Pn

Typeset using REVTeX

I. INTRODUCTION

We have recently shown [1] that the stochastic selection of the correlated Gaussian [2,3] basis functions leads to precise variational solutions for diverse fermionic and bosonic nonadiabatic $N = 2 - 7$ -body systems. The trial function in a variational approach must be flexible enough to describe the full variety of correlations between the particles. The correlation is conveniently represented by a correlation factor, $F = \prod_{i < j}^N f_{ij}$, and thus the trial function is often chosen to be of this form. The trial function of Hylleraas type, which is used in atomic and molecular physics, approximates f_{ij} as a linear combination of exponentials, $\exp[-\alpha_{ij}|\mathbf{r}_i - \mathbf{r}_j|]$. If f_{ij} is approximated as a linear combination of Gaussians, $\exp[-\alpha_{ij}(\mathbf{r}_i - \mathbf{r}_j)^2]$, the N -particle trial function then contains a product of these Gaussians: $\prod_{i < j}^N \exp[-\alpha_{ij}(\mathbf{r}_i - \mathbf{r}_j)^2] = \exp[-\sum_{i < j}^N \alpha_{ij}(\mathbf{r}_i - \mathbf{r}_j)^2]$ [4-6].

The above form of the correlated function describes the motion with the orbital angular momentum $L = 0$ only. It is obviously important to extend the correlated function to the case with $L > 0$, and in fact there is an increasing interest in finding a precise solution with $L \geq 2$ for the Coulomb three-body systems [7]. The standard way to describe the rotational motion is to vectorially couple the solid spherical harmonics of the relative coordinates [7,8]. Each of the solid spherical harmonics carries the partial wave for the corresponding relative motion. Since these partial waves are in general not good quantum numbers, several sets of partial waves are in general necessary for a realistic description of the motion, particularly in a nuclear system [9,10]. Another way to incorporate the angular dependence is to use Cartesian Gaussian functions. The calculation of matrix elements becomes complicated in both cases, especially when the number of particles increases or high angular momenta are involved. A quite different way to introduce the angular part, proposed in [1], involves no partial wave decomposition for each relative motion but attempts to determine a vector which has closest relevance to the rotational motion. The vector is defined as a linear combination of the relative coordinates and their coefficients can be treated as variational parameters. The formulation using this new angular part is entirely free from the complexity involved in the angular momentum coupling.

The purpose of this paper is to exploit this formulation in greater detail, to present the formulas needed for N -body system interacting via central force, and to test its utility by applying to Coulomb three-body problems such as the muonic molecule and the helium atom. Several authors have investigated both the ground and excited states of these systems, for example in [8,11-14] for the muonic molecule and in [15,16] for the helium atom. A comparison with the solutions known in literature will be useful to judge the utility of the present formulation. Although any spherically symmetric orbital functions can be used together with the angular part introduced here, the correlated Gaussian has the advantage of simplicity in the coordinate transformation.

In section II we introduce the correlated Gaussian with the angular momentum dependence and show that the matrix elements can easily be evaluated with the use of the generating function of the correlated Gaussian. No problem arises as to the center-of-mass motion because the formalism does not include any dependence on the center-of-mass variable. In section III some of the results for the Coulomb three-body system are presented within the new formulation for the angular dependence and compared to those available in literature. A summary is given in section IV.

II. FORMALISM

A. The correlated Gaussians

Any square-integrable function with angular momentum lm can be approximated, to any desired accuracy, by a linear combination of nodeless harmonic-oscillator functions (Gaussians) of continuous size parameter a [17]:

$$\Gamma_{lm}(\mathbf{r}) \sim e^{-\frac{1}{2}ar^2} \mathcal{Y}_{lm}(\mathbf{r}), \quad \text{with} \quad \mathcal{Y}_{lm}(\mathbf{r}) = |\mathbf{r}|^l Y_{lm}(\hat{\mathbf{r}}). \quad (1)$$

A generalization of this to N -particle systems contains a product of the Gaussians $\exp[-\sum_{i<j}^N \alpha_{ij}(\mathbf{r}_i - \mathbf{r}_j)^2]$. The product can be conveniently expressed in terms of a set of $(N-1)$ independent relative coordinates \mathbf{x} , $(\mathbf{x}_1, \dots, \mathbf{x}_{N-1})$, instead of $N(N-1)/2$ interparticle distance vectors $(\mathbf{r}_i - \mathbf{r}_j)$. By a set of relative coordinates we mean the one in which the intrinsic kinetic energy operator takes the form $\sum_{i=1}^{N-1} \mathbf{p}_i^2/2\mu_i$ with reduced masses μ_i . Even with this condition there are a number of possible sets of relative coordinates. One can choose, however, any one of the sets as \mathbf{x} because each set of relative coordinates is obtained from any other set of relative coordinates by an appropriate $(N-1) \times (N-1)$ matrix T . The relative coordinates are assumed to be normalized in such a way that the volume element remains unchanged under the coordinate transformation, which requires that the determinant of T is unity. An N -particle basis function, the so-called correlated Gaussian, then looks like

$$\psi_{LM}(A, \mathbf{x}) = e^{-\frac{1}{2}\tilde{\mathbf{x}}A\mathbf{x}} \theta_{LM}(\mathbf{x}), \quad (2)$$

where A is an $(N-1) \times (N-1)$ positive-definite, symmetric matrix containing $N(N-1)/2$ nonlinear parameters, specific to each basis element, and the quadratic form, $\tilde{\mathbf{x}}A\mathbf{x}$, involves scalar products of the Cartesian vectors: $\tilde{\mathbf{x}}A\mathbf{x} = \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} A_{ij} \mathbf{x}_i \cdot \mathbf{x}_j$.

The function $\theta_{LM}(\mathbf{x})$ in Eq. (2), which represents the angular part of the wave function with the total orbital angular momentum L and its projection M , is a generalization of \mathcal{Y} in Eq. (1). Usually it is chosen as a vector-coupled product of solid spherical harmonics of the relative coordinates

$$\theta_{LM}(\mathbf{x}) = [[[\mathcal{Y}_{l_1}(\mathbf{x}_1)\mathcal{Y}_{l_2}(\mathbf{x}_2)]_{L_{12}}\mathcal{Y}_{l_3}(\mathbf{x}_3)]_{L_{123}}\dots]_{LM}, \quad (3)$$

where the square bracket stands for the coupling of angular momenta. Each relative motion has a definite angular momentum in Eq. (3). Since the set of angular momenta itself is not a conserved quantity, it may be important to include several sets of angular momenta $(l_1, l_2, \dots, l_{N-1}; L_{12}, L_{123}, \dots)$ for a realistic description. This is the case especially in nuclear few-body problems [9,10,18]. It is also noted that a faster convergence is in general obtained by allowing the use of different sets of relative coordinates together with suitable sets of angular momenta. From the fact that $\theta_{LM}(\mathbf{x})$ can be expressed by different partial wave decompositions in different relative coordinate systems, one can conclude that the usage of partial waves may not be so important after all. Besides, the various possible partial wave contributions increase the basis dimension. Moreover, the calculation of matrix elements for this choice of $\theta_{LM}(\mathbf{x})$ sooner or later becomes too complicated. This choice is therefore

apparently inconvenient especially as the number of particles increases and/or the different sets of relative coordinates are employed.

As proposed in [1], this difficulty can be avoided by adopting a different choice for $\theta_{LM}(\mathbf{x})$:

$$\theta_{LM}(\mathbf{x}) = \eta_{KLM}(u, \mathbf{x}) = |\mathbf{v}|^{2K+L} Y_{LM}(\hat{\mathbf{v}}), \quad \text{with} \quad \mathbf{v} = \sum_{i=1}^{N-1} u_i \mathbf{x}_i = \tilde{u} \mathbf{x}. \quad (4)$$

Only the total orbital angular momentum, which is (at least approximately) a good quantum number in most cases, appears in this expression. The real vector $\tilde{u} = (u_1, \dots, u_{N-1})$ defines a global vector, \mathbf{v} , a linear combination of the relative coordinates, and the wave function of the system is expanded in terms of its angle $\hat{\mathbf{v}}$. The vector u may be considered a variational parameter and one may try to minimize the energy functional with respect to it. The energy minimization then amounts to finding the most suitable angle or a linear combination of angles. The continuity of the parameter u can be more advantageous in a variational calculation than the discrete nature of the set of the angular momenta $(l_1, l_2, \dots, l_{N-1}; L_{12}, L_{123}, \dots)$ because the change of the energy functional can be continuously seen in the former case. The factor of $|\mathbf{v}|^{2K+L}$ plays an important role in improving the short-range behavior of the wave function, e.g., the Coulomb cusp ratio [19]. A remarkable advantage of this form of $\theta_{LM}(\mathbf{x})$ is that the calculation of matrix elements becomes much simpler than in the former case because the coupling of $(N-1)$ angular momenta is completely avoided.

The two forms of $\theta_{LM}(\mathbf{x})$ are in fact closely related to each other. It is easy to see that any of the functions of Eq. (4) is a linear combination of the terms of Eq. (3), each multiplied by an appropriate monomial of the variables, $\mathbf{x}_1^2, \dots, \mathbf{x}_{N-1}^2$. For example, it takes a particularly simple form for the three-body system, i.e., for the vector $\mathbf{v} = u_1 \mathbf{x}_1 + u_2 \mathbf{x}_2$

$$\begin{aligned} |\mathbf{v}|^{2K+L} Y_{LM}(\hat{\mathbf{v}}) &= \sqrt{4\pi} \sum_{\substack{k_1, l_1, k_2, l_2 \geq 0 \\ 2k_1 + l_1 + 2k_2 + l_2 = 2K+L}} u_1^{2k_1+l_1} u_2^{2k_2+l_2} \\ &\times \frac{(2K)!!(2K+2L+1)!!}{(2k_1)!!(2k_1+2l_1+1)!!(2k_2)!!(2k_2+2l_2+1)!!} \sqrt{\frac{(2l_1+1)(2l_2+1)}{2L+1}} \langle l_1 0 l_2 0 | L 0 \rangle \\ &\times |\mathbf{x}_1|^{2k_1} |\mathbf{x}_2|^{2k_2} [\mathcal{Y}_{l_1}(\mathbf{x}_1) \mathcal{Y}_{l_2}(\mathbf{x}_2)]_{LM}. \end{aligned} \quad (5)$$

Table I lists possible sets of k_1, l_1, k_2 , and l_2 values for small K and L values. In the case of $K = 0$ both k_1 and k_2 are limited to zero and only the stretched coupling, namely $l_1 + l_2 = L$, is allowed. With an increasing K value the possible values of partial waves l_1 and l_2 increase including the case of non-stretched coupling. To increase K is thus one way to include higher partial waves in the calculation. Note, however, that even with $K = 0$ additional and important partial wave contribution comes from the cross term of the exponential part of the correlated Gaussian if A is not diagonal. Conversely any two-variable functions of Eq. (3) with natural parity, i.e., $(-1)^{l_1+l_2} = (-1)^L$, may be expressed in terms of a linear combination of the terms, $|\mathbf{v}|^{2K+L} Y_{LM}(\hat{\mathbf{v}})$, by using some appropriate sets of u values, each multiplied by a monomial of degree $l_1 + l_2 - 2K - L$ in \mathbf{x}_1^2 and \mathbf{x}_2^2 . See Appendix for the details. A generalization of the argument in Appendix will lead to a conclusion that some functions of Eq. (3) may be given in terms of a linear combination of Eq. (4), each multiplied by the terms such as \mathbf{x}_i^2 and $(\mathbf{x}_i \cdot \mathbf{x}_j)$. Namely, the rotational property of the function of Eq. (3) may be represented by combinations of simple forms of Eq. (4). Therefore, if one can

calculate the matrix elements using $\theta_{LM}(\mathbf{x})$ defined in Eq. (4), then those with the previous form of $\theta_{LM}(\mathbf{x})$ of certain class can be obtained readily.

The correlated Gaussian we proposed is thus given by

$$f_{KLM}(u, A, \mathbf{x}) = \eta_{KLM}(u, \mathbf{x}) e^{-\frac{1}{2} \tilde{\mathbf{x}} A \mathbf{x}}. \quad (6)$$

A useful property of the function f is its form-invariance with respect to the transformation of the coordinates \mathbf{x} to any other set of coordinates \mathbf{y} , that is, for $\mathbf{x} = T\mathbf{y}$,

$$f_{KLM}(u, A, \mathbf{x}) = f_{KLM}(u', A', \mathbf{y}), \quad (7)$$

with

$$A' = \tilde{T} A T, \quad u' = \tilde{T} u. \quad (8)$$

Here \tilde{T} is the transpose of T . As will be seen later, this property is fully exploited in evaluating the matrix elements. It is necessary to impose a proper permutation symmetry on the basis states for the system of identical particles. The symmetry requirement causes a linear transformation of the coordinates, and it can easily be incorporated in the present formulation thanks to the form-invariance of the correlated Gaussian mentioned above. It would be rather complicated to construct the symmetry-adapted basis states using the angular function of Eq. (3).

The calculation of the matrix elements becomes simpler if one uses a generating function of the correlated Gaussian. In fact, the following function g is found to be convenient to generate the function f [1]:

$$f_{KLM}(u, A, \mathbf{x}) = \frac{1}{B_{KL}} \int d\hat{\mathbf{t}} Y_{LM}(\hat{\mathbf{t}}) \left(\frac{d^{2K+L}}{d\alpha^{2K+L}} g(\alpha, \mathbf{t}; u, A, \mathbf{x}) \right)_{\substack{\alpha=0 \\ t=|\mathbf{t}|=1}}, \quad (9)$$

where

$$g(\alpha, \mathbf{t}; u, A, \mathbf{x}) = e^{-\frac{1}{2} \tilde{\mathbf{x}} A \mathbf{x} + \alpha \mathbf{t} \cdot (\tilde{u} \mathbf{x})}, \quad (10)$$

$$B_{nl} = \frac{4\pi(2n+l)!}{2^n n! (2n+2l+1)!!}. \quad (11)$$

Here \mathbf{t} is a unit vector. Equation (9) is easily proved by using the simple formula

$$(\mathbf{a} \cdot \mathbf{b})^k = |\mathbf{a}|^k |\mathbf{b}|^k \sum_{\substack{n,l \geq 0 \\ 2n+l=k}} B_{nl} \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{a}}) Y_{lm}(\hat{\mathbf{b}})^*. \quad (12)$$

The correlated Gaussian basis of Eq. (6) has parity $(-1)^L$. To construct a function with parity $(-1)^{L+1}$, the angular part of Eq. (6) must be slightly modified, e.g., to

$$\theta_{LM}(\mathbf{x}) = [\eta_{KL}(u, \mathbf{x}) \eta_{01}(u', \mathbf{x})]_{LM}. \quad (13)$$

In this case the generating function g of Eq. (10) must be modified to include another factor $\alpha' \mathbf{t}' \cdot (\tilde{u}' \mathbf{x})$. Equation (9) is then extended to

$$\begin{aligned} & [\eta_{KL}(u, \mathbf{x}) \eta_{01}(u', \mathbf{x})]_{LM} e^{-\frac{1}{2} \tilde{\mathbf{x}} A \mathbf{x}} \\ &= \frac{1}{B_{KL} B_{01}} \int \int d\hat{\mathbf{t}} d\hat{\mathbf{t}}' [Y_L(\hat{\mathbf{t}}) Y_1(\hat{\mathbf{t}}')]_{LM} \left(\frac{d^{2K+L+1}}{d\alpha^{2K+L} d\alpha'} e^{-\frac{1}{2} \tilde{\mathbf{x}} A \mathbf{x} + \alpha \mathbf{t} \cdot (\tilde{u} \mathbf{x}) + \alpha' \mathbf{t}' \cdot (\tilde{u}' \mathbf{x})} \right)_{\substack{\alpha=\alpha'=0 \\ t=t'=1}}. \end{aligned} \quad (14)$$

B. Calculation of the matrix elements

In this subsection we will give the details of the method of calculating the matrix elements between the basis function of Eq. (6). One can already see some useful formulas for $L = 0$ motion in [4,6]. The aim here is to demonstrate that the matrix elements for arbitrary L can be obtained as simply as those for $L = 0$. As will be seen later, one generally needs the matrix elements of the two functions which are expressed in terms of different sets of relative coordinates.

The overlap matrix element is obtained as

$$\begin{aligned} \langle f_{KLM}(u, A, \mathbf{y}) | f_{K'LM}(v, B, \mathbf{x}) \rangle &= \langle f_{KLM}(u, A, \mathbf{y}) | f_{K'LM}(v', B', \mathbf{y}) \rangle \\ &= \frac{1}{B_{KL}B_{K'L}} \int \int d\hat{\mathbf{t}} d\hat{\mathbf{t}}' Y_{LM}(\hat{\mathbf{t}})^* Y_{LM}(\hat{\mathbf{t}}') \\ &\quad \times \left(\frac{d^{\kappa+\kappa'}}{d\alpha^\kappa d\alpha'^{\kappa'}} \left(\frac{(2\pi)^{N-1}}{\det C} \right)^{3/2} e^{p\alpha^2 + p'\alpha'^2 + q\alpha\alpha' \mathbf{t} \cdot \mathbf{t}'} \right)_{\substack{\alpha=\alpha'=0 \\ t=t'=1}}, \end{aligned} \quad (15)$$

with an abbreviation

$$\kappa = 2K + L, \quad \kappa' = 2K' + L, \quad (16)$$

where the property of Eq. (7) is used and where

$$C = A + B', \quad p = \frac{1}{2} \tilde{u} C^{-1} u, \quad p' = \frac{1}{2} \tilde{v}' C^{-1} v', \quad q = \frac{1}{2} \left(\tilde{u} C^{-1} v' + \tilde{v}' C^{-1} u \right). \quad (17)$$

Here we used the familiar formula of the $3n$ -dimensional Gaussian integration

$$\int d\mathbf{x} e^{-\frac{1}{2} \tilde{\mathbf{x}} A \mathbf{x} + \tilde{\mathbf{T}} \mathbf{x}} = \left(\frac{(2\pi)^n}{\det A} \right)^{3/2} e^{\frac{1}{2} \tilde{\mathbf{T}} A^{-1} \mathbf{T}}, \quad (18)$$

where A is an $n \times n$ symmetric matrix and $\tilde{\mathbf{T}} = (\mathbf{T}_1, \dots, \mathbf{T}_n)$ is a row vector comprising three-dimensional vectors \mathbf{T}_i . Differentiating with respect to α and α' , followed by $\alpha = \alpha' = 0$, and integrating over the angles of \mathbf{t} and \mathbf{t}' leads us to

$$\begin{aligned} \langle f_{KLM}(u, A, \mathbf{y}) | f_{K'LM}(v, B, \mathbf{x}) \rangle &= \frac{1}{B_{KL}B_{K'L}} \left(\frac{(2\pi)^{N-1}}{\det C} \right)^{3/2} \kappa! \kappa'! \sum_{n=0}^{\min(K, K')} \frac{p^{K-n} p'^{K'-n} q^{L+2n}}{(K-n)!(K'-n)!(L+2n)!} B_{nL}. \end{aligned} \quad (19)$$

The matrix element of the kinetic energy operator is calculated in a similar way. Expressing the intrinsic kinetic energy operator in terms of the set of coordinates \mathbf{y} of the bra side, we obtain

$$\begin{aligned} \langle f_{KLM}(u, A, \mathbf{y}) | \sum_{i=1}^{N-1} \frac{\mathbf{p}_i^2}{2\mu_i} | f_{K'LM}(v, B, \mathbf{x}) \rangle &= \langle f_{KLM}(u, A, \mathbf{y}) | \sum_{i=1}^{N-1} \frac{\mathbf{p}_i^2}{2\mu_i} | f_{K'LM}(v', B', \mathbf{y}) \rangle \\ &= \frac{1}{B_{KL}B_{K'L}} \int \int d\hat{\mathbf{t}} d\hat{\mathbf{t}}' Y_{LM}(\hat{\mathbf{t}})^* Y_{LM}(\hat{\mathbf{t}}') \left(\frac{d^{\kappa+\kappa'}}{d\alpha^\kappa d\alpha'^{\kappa'}} \langle g(\alpha, \mathbf{t}, u, A, \mathbf{y}) | \right. \\ &\quad \times \left[3\text{Tr} \Lambda B' - \alpha'^2 \tilde{v}' \Lambda v' + 2\alpha' \mathbf{t}' \cdot (\tilde{v}' \Lambda B' \mathbf{y}) - \tilde{\mathbf{y}} B' \Lambda B' \mathbf{y} \right] | g(\alpha', \mathbf{t}', v', B', \mathbf{y}) \rangle \Bigg)_{\substack{\alpha=\alpha'=0 \\ t=t'=1}}. \end{aligned} \quad (20)$$

Here Λ is an $(N-1) \times (N-1)$ diagonal matrix

$$\Lambda = \begin{pmatrix} \frac{\hbar^2}{2\mu_1} & 0 & \dots & 0 \\ 0 & \frac{\hbar^2}{2\mu_2} & & \vdots \\ \vdots & & & \vdots \\ 0 & \dots & \dots & \frac{\hbar^2}{2\mu_{N-1}} \end{pmatrix}. \quad (21)$$

The integration over \mathbf{y} in Eq. (20) can be done by using the formula of Eq. (18) as follows:

$$\begin{aligned} \int d\mathbf{x} \tilde{\mathbf{U}}\mathbf{x} e^{-\frac{1}{2}\tilde{\mathbf{x}}A\mathbf{x}+\tilde{\mathbf{T}}\mathbf{x}} &= \left(\frac{d}{d\alpha} \int d\mathbf{x} e^{-\frac{1}{2}\tilde{\mathbf{x}}A\mathbf{x}+(\tilde{\mathbf{T}}+\alpha\tilde{\mathbf{U}})\mathbf{x}} \right)_{\alpha=0} \\ &= \left(\frac{(2\pi)^n}{\det A} \right)^{3/2} \frac{1}{2} (\tilde{\mathbf{U}}A^{-1}\mathbf{T} + \tilde{\mathbf{T}}A^{-1}\mathbf{U}) e^{\frac{1}{2}\tilde{\mathbf{T}}A^{-1}\mathbf{T}}, \end{aligned} \quad (22)$$

$$\begin{aligned} \int d\mathbf{x} \tilde{\mathbf{x}}B\mathbf{x} e^{-\frac{1}{2}\tilde{\mathbf{x}}A\mathbf{x}+\tilde{\mathbf{T}}\mathbf{x}} &= \left(-2\frac{d}{d\alpha} \int d\mathbf{x} e^{-\frac{1}{2}\tilde{\mathbf{x}}(A+\alpha B)\mathbf{x}+\tilde{\mathbf{T}}\mathbf{x}} \right)_{\alpha=0} \\ &= \left(\frac{(2\pi)^n}{\det A} \right)^{3/2} (3\text{Tr}A^{-1}B + \tilde{\mathbf{T}}A^{-1}BA^{-1}\mathbf{T}) e^{\frac{1}{2}\tilde{\mathbf{T}}A^{-1}\mathbf{T}}. \end{aligned} \quad (23)$$

Using Eqs. (22) and (23) in Eq. (20) leads us to

$$\begin{aligned} &\langle f_{KLM}(u, A, \mathbf{y}) | \sum_{i=1}^{N-1} \frac{\mathbf{p}_i^2}{2\mu_i} | f_{K'LM}(v, B, \mathbf{x}) \rangle \\ &= \frac{1}{B_{KL}B_{K'L}} \int \int d\hat{\mathbf{t}} d\hat{\mathbf{t}}' Y_{LM}(\hat{\mathbf{t}})^* Y_{LM}(\hat{\mathbf{t}}') \left(\frac{d^{\kappa+\kappa'}}{d\alpha^\kappa d\alpha'^{\kappa'}} \right. \\ &\quad \times \left. \left(\frac{(2\pi)^{N-1}}{\det C} \right)^{3/2} [R + P\alpha^2 + P'\alpha'^2 + Q\alpha\alpha'\mathbf{t} \cdot \mathbf{t}'] e^{p\alpha^2 + p'\alpha'^2 + q\alpha\alpha'\mathbf{t} \cdot \mathbf{t}'} \right)_{\substack{\alpha=\alpha'=0 \\ t=t'=1}}, \end{aligned} \quad (24)$$

where

$$\begin{aligned} R &= 3\text{Tr}\Lambda B'C^{-1}A, \quad P = -\tilde{u}C^{-1}B'\Lambda B'C^{-1}u, \quad P' = -\tilde{v}'C^{-1}A\Lambda AC^{-1}v', \\ Q &= \tilde{u}C^{-1}B'\Lambda AC^{-1}v' + \tilde{v}'C^{-1}A\Lambda B'C^{-1}u. \end{aligned} \quad (25)$$

The matrix element of the kinetic energy operator is finally obtained as

$$\begin{aligned} &\langle f_{KLM}(u, A, \mathbf{y}) | \sum_{i=1}^{N-1} \frac{\mathbf{p}_i^2}{2\mu_i} | f_{K'LM}(v, B, \mathbf{x}) \rangle \\ &= \frac{1}{B_{KL}B_{K'L}} \left(\frac{(2\pi)^{N-1}}{\det C} \right)^{3/2} \kappa! \kappa'! \sum_{n=0}^{\min(K, K')} \\ &\quad \times [Rpp'q + (K-n)Pp'q + (K'-n)pP'q + (L+2n)pp'Q] \\ &\quad \times \frac{p^{K-n-1}p'^{K'-n-1}q^{L+2n-1}}{(K-n)!(K'-n)!(L+2n)!} B_{nL}. \end{aligned} \quad (26)$$

The present formulation does not have any problem arising from the center-of-mass motion as discussed in [4,5].

We will show the evaluation of the potential energy matrix element by assuming that the potential V_{ij} is a function of the distance $|\mathbf{r}_i - \mathbf{r}_j|$ only. There is at least one set of coordinates, say, \mathbf{z} , in which $(\mathbf{r}_i - \mathbf{r}_j)$ can be chosen to be \mathbf{z}_1 . It is then convenient to calculate the matrix element of the potential by transforming both of the correlated Gaussians on bra and ket sides to those expressed in this set of coordinates:

$$\begin{aligned} \langle f_{KLM}(u, A, \mathbf{y}) | V_{ij} | f_{K'LM}(v, B, \mathbf{x}) \rangle &= \langle f_{KLM}(u', A', \mathbf{z}) | V(z_1) | f_{K'LM}(v', B', \mathbf{z}) \rangle \\ &= \frac{1}{B_{KL} B_{K'L}} \int \int d\hat{\mathbf{t}} d\hat{\mathbf{t}}' Y_{LM}(\hat{\mathbf{t}})^* Y_{LM}(\hat{\mathbf{t}}') \\ &\quad \times \left(\frac{d^{\kappa+\kappa'}}{d\alpha^\kappa d\alpha'^{\kappa'}} \langle g(\alpha, \mathbf{t}, u', A', \mathbf{z}) | V(z_1) | g(\alpha', \mathbf{t}', v', B', \mathbf{z}) \rangle \right)_{\substack{\alpha=\alpha'=0 \\ \hat{\mathbf{t}}=\hat{\mathbf{t}}'=1}}, \end{aligned} \quad (27)$$

where A' and u' are defined by Eq. (8) with the matrix T corresponding to the $\mathbf{y} \rightarrow \mathbf{z}$ transformation $\mathbf{y} = T\mathbf{z}$, while B' and v' are obtained similarly by the matrix corresponding to the $\mathbf{x} \rightarrow \mathbf{z}$ transformation.

To perform the integration over \mathbf{z} in Eq. (27) we introduce the short-hand notation as follows:

$$\begin{aligned} \tilde{u}' &= (u'_1, u'_2, \dots, u'_{N-1}) = (u'_1, \tilde{\omega}), & \tilde{v}' &= (v'_1, v'_2, \dots, v'_{N-1}) = (v'_1, \tilde{\chi}), \\ A' + B' &= \begin{pmatrix} c & \gamma_1 & \dots & \gamma_{N-2} \\ \gamma_1 & & & \\ \vdots & & \Gamma & \\ \gamma_{N-2} & & & \end{pmatrix}. \end{aligned} \quad (28)$$

By introducing $\tilde{\gamma} = (\gamma_1, \dots, \gamma_{N-2})$ and $\tilde{\mathbf{z}} = (\mathbf{z}_1, \dots, \mathbf{z}_{N-1}) = (\mathbf{z}_1, \tilde{\mathbf{w}})$, the \mathbf{z} integration of Eq. (27) becomes

$$\begin{aligned} \langle g(\alpha, \mathbf{t}, u', A', \mathbf{z}) | V(z_1) | g(\alpha', \mathbf{t}', v', B', \mathbf{z}) \rangle &= \int \int d\mathbf{z}_1 d\mathbf{w} V(z_1) \\ &\quad \times \exp\left(-\frac{1}{2}c z_1^2 + (\alpha u'_1 \mathbf{t} + \alpha' v'_1 \mathbf{t}') \cdot \mathbf{z}_1 - \frac{1}{2} \tilde{\mathbf{w}} \Gamma \mathbf{w} + [\alpha \mathbf{t} \cdot (\tilde{\omega} \mathbf{w}) + \alpha' \mathbf{t}' \cdot (\tilde{\chi} \mathbf{w}) - \mathbf{z}_1 \cdot (\tilde{\gamma} \mathbf{w})]\right) \\ &= \left(\frac{(2\pi)^{N-2}}{\det \Gamma} \right)^{3/2} e^{p_v \alpha^2 + p'_v \alpha'^2 + q_v \alpha \alpha' \mathbf{t} \cdot \mathbf{t}'} \int d\mathbf{z}_1 V(z_1) e^{-\frac{1}{2}(c - \tilde{\gamma} \Gamma^{-1} \gamma) z_1^2 + (\lambda \alpha \mathbf{t} + \lambda' \alpha' \mathbf{t}') \cdot \mathbf{z}_1} \\ &= \left(\frac{(2\pi)^{N-2}}{\det \Gamma} \right)^{3/2} e^{p_v \alpha^2 + p'_v \alpha'^2 + q_v \alpha \alpha' \mathbf{t} \cdot \mathbf{t}'} 4\pi \int_0^\infty dz_1 z_1^2 V(z_1) e^{-\frac{1}{2}(c - \tilde{\gamma} \Gamma^{-1} \gamma) z_1^2} i_0(|\lambda \alpha \mathbf{t} + \lambda' \alpha' \mathbf{t}'| z_1). \end{aligned} \quad (29)$$

where

$$\begin{aligned} p_v &= \frac{1}{2} \tilde{\omega} \Gamma^{-1} \omega, & p'_v &= \frac{1}{2} \tilde{\chi} \Gamma^{-1} \chi, & q_v &= \frac{1}{2} \left(\tilde{\omega} \Gamma^{-1} \chi + \tilde{\chi} \Gamma^{-1} \omega \right), \\ \lambda &= u'_1 - \frac{1}{2} \left(\tilde{\gamma} \Gamma^{-1} \omega + \tilde{\omega} \Gamma^{-1} \gamma \right), & \lambda' &= v'_1 - \frac{1}{2} \left(\tilde{\gamma} \Gamma^{-1} \chi + \tilde{\chi} \Gamma^{-1} \gamma \right), \end{aligned} \quad (30)$$

and $i_0(x) = \sinh x/x$. Substituting Eq. (29) into Eq. (27), followed by a power series expansion of $i_0(x)$, and doing the needed operation leads us to

$$\begin{aligned} & \langle f_{KLM}(u, A, \mathbf{y}) | V(z_1) | f_{K'LM}(v, B, \mathbf{x}) \rangle \\ &= \frac{1}{B_{KL}B_{K'L}} \left(\frac{(2\pi)^{N-2}}{\det\Gamma} \right)^{3/2} \kappa! \kappa'! \sum_{m=0}^{K+K'+L} \sum_{i=0}^m \sum_{j=0}^{m-i} \sum_{n=\max(0, \frac{m-i-j-L}{2})}^{\min(K-i, K'-j)} I(2m+2, c - \gamma\Gamma^{-1}\gamma) \\ & \times \frac{2^{m-i-j} m! \lambda^{m+i-j} \lambda'^{m-i+j} p_v^{K-i-n} p_v'^{K'-j-n} q_v^{L+2n-m+i+j}}{(2m+1)! i! j! (m-i-j)! (K-i-n)! (K'-j-n)! (L+2n-m+i+j)!} B_{nL}, \end{aligned} \quad (31)$$

with

$$I(n, a) = 4\pi \int_0^\infty dz_1 V(z_1) z_1^n e^{-\frac{1}{2}az_1^2}. \quad (32)$$

The integral of Eq. (32) becomes elementary for the Coulomb potential. The calculation of the mean distance, the root mean square distance or the mean inverse distance between the particles can easily be done by putting $V(z) = z$, z^2 or $1/z$ in the above integral.

The calculation of the matrix elements described above is much simpler than the case where the function $\theta_{LM_L}(\mathbf{x})$ is decomposed into partial waves of the relative coordinates as in Eq. (3). In fact, in that latter case one has to integrate over the angles of the relative coordinates and one has to cope with the angular momentum algebra. We note, however, that the calculation of the matrix element of the latter type poses no problem if the function $\theta_{LM_L}(\mathbf{x})$ of Eq. (3) is expressed as a linear combination of the terms of Eq. (4) with appropriate u -vectors. It is appealing that the present formalism does not require any modification with respect to an increasing N .

All the matrix elements can be given in a closed analytic form and the numerical evaluation of the matrix elements as a function of the nonlinear parameters is therefore straightforward. The values, $\kappa = 2K+L$ and $\kappa' = 2K'+L$, are usually small in practical cases and the sum in Eqs. (19), (26), and (31) is limited to just a few terms.

The partial derivative of matrix elements with respect to variational parameters may sometimes be useful when one searches for an optimal set of parameters. Since the dependence on the parameters is explicitly given for the matrix elements of the correlated Gaussians, it would not be difficult to derive the expression for the derivative. As stated in the previous section, the u -vector is considered a variational parameter which defines the most suitable global vector to describe the rotational motion. The calculation of the derivative of the matrix elements with respect to u_i is particularly simple because of the simple structure of the u -dependence. It can also be calculated by using an equation analogous to Eq. (14) because the derivative of η_{KLM} with respect to u_i is expressed as a tensor product of two η 's as follows:

$$\begin{aligned} \frac{\partial}{\partial u_i} \eta_{KLM}(u, \mathbf{x}) &= (2K+2L+1) \sqrt{\frac{L}{2L+1}} [\eta_{KL-1}(u, \mathbf{x}) \mathbf{x}_i]_{LM} \\ &\quad - 2K \sqrt{\frac{L+1}{2L+1}} [\eta_{K-1L+1}(u, \mathbf{x}) \mathbf{x}_i]_{LM}. \end{aligned} \quad (33)$$

Note that \mathbf{x}_i is equal to $\sqrt{4\pi/3} \eta_{01}(u', \mathbf{x})$ with u' being defined by $u'_j = \delta_{ij}$.

III. SPECIFIC EXAMPLES: COULOMB THREE-BODY SYSTEM

This section is devoted to show the bound-state solutions of Coulomb three-body problems by using the method described above. To test the method we consider the positronium negative ion $e^-e^-e^+$, the muonic molecules of $tt\mu^-$ and $td\mu^-$, and the helium atom αe^-e^- . These systems are chosen because they cover a wide range of mass ratio of the constituent particles and include some rotational bound states: The positronium negative ion consists of particles of identical mass, which makes it difficult to treat the system in an adiabatic approach, the mass of t or d in the muonic molecule is a few ten times heavier than the mass of μ , and in the helium atom the mass of the heavy particle is several thousand times larger than the e^- mass, which is the realm of the adiabatic approach. One can in principle consider other systems with the method, but there are already highly accurate calculations available for the above systems. We assume that the orbital wave function is antisymmetric with respect to the interchange of the two identical particles except for the case of the spin-singlet states of the helium atom.

The trial wave function is chosen to be a linear combination of the correlated Gaussian of type (6). Without loss of generality the vector u can be set to satisfy $u_1^2 + u_2^2 = 1$. Each basis function thus contains at most four nonlinear parameters, three of which come from the matrix A . To assure the positive definiteness of the correlated Gaussians, A can in general be expressed as $A = \tilde{G}DG$ [5], where G is an $(N-1) \times (N-1)$ orthogonal matrix containing $(N-1)(N-2)/2$ parameters and D is a diagonal matrix, $D_{ij} = d_i\delta_{ij}$, including $(N-1)$ positive parameters d_i . Although no restriction on the parameters of the matrix G is in principle necessary, it is advisable to avoid too many variables if possible. The most naive choice would be to take G as a unit matrix, which is equivalent to using only a single set of coordinates \mathbf{x} , and then to try to reach convergence by including successively higher partial waves implied by an appropriate choice of K and u values. Many examples show [1,8,18], however, that this type of single channel calculations does not work well especially in those systems where the adiabatic approximation of the motion is questionable because the various types of correlated motion become important. Instead the matrix A may be chosen as $A = \widetilde{T^{-1}}DT^{-1}$, where T is such a matrix that connects the coordinates \mathbf{x} to an arbitrary set of relative coordinates \mathbf{y} , $\mathbf{x} = T\mathbf{y}$. In this case $\tilde{\mathbf{x}}A\mathbf{x}$ becomes $\tilde{\mathbf{y}}D\mathbf{y} = \sum_{i=1}^{N-1} d_i y_i^2$. The Gaussians with this choice of A together with the angular part of Eq. (3) have recently been shown to give a precise solution for few-nucleon systems with realistic nucleon-nucleon potentials including noncentral components [10]. Since our interest is to test the utility of Eq. (6), we restricted the choice of A and a maximum value of K to the following three simple cases:

- (i) $K_{\max} = 0$ and $A = \widetilde{T^{-1}}DT^{-1}$, where T represents a special matrix connecting to three sets of relative coordinates (the so-called rearrangement channels) and D is diagonal.
- (ii) $K_{\max} = 1$ and the choice of A is the same as in case (i).
- (iii) $K_{\max} = 0$ but A is an arbitrary positive-definite, symmetric matrix.

In case (iii) the matrix A can be parametrized as $A = \tilde{G}DG$ with an orthogonal matrix G . As was already mentioned in the previous section, the angular part with $K = 0$ describes

the stretched configuration and therefore allows such limited angular correlations in case (i). The case (ii) is an extension of this case to include the non-stretched coupling. The angular correlation between the particles is taken into account in case (iii) by the cross term of the exponential part of the correlated Gaussian.

Our primary purpose is to investigate if our basis functions with the new angular part can universally yield satisfactory results of the same quality independently of the system. Results of the calculation presented below are thus limited up to the maximum basis dimension $\mathcal{K} = 200$ for all the systems. With a larger basis size one can definitely obtain much more accurate results but this is beyond our purpose. Even with $\mathcal{K} = 200$ dimension there are a large number of nonlinear parameters. A complete optimization is in principle superior to any other method but it is neither practical nor possible at present. Instead we select the basis elements in the trial function stepwise according to the stochastic variational method (SVM) [1,20,21,18,10]. The SVM attempts to select the most appropriate basis elements in a trial and error procedure: Various randomly generated candidates for the basis element are tested and the usefulness of these states are judged by their contribution to the energy of the system. The SVM has proved to provide a precise solution for various few-body systems with a reasonable computational effort. The refining procedure employed in [10] to tune the nonlinear parameters was effective to reach the solution of high quality for three- and four-nucleon systems interacting with realistic nuclear potentials and was successfully used in the present paper as well. The basis selection in the SVM can be done by exploiting the special form of the Hamiltonian matrix as shown in Ref. [1] and it does not carry heavy computational loads. There are several sophisticated optimization strategies in quantum chemistry [3,6,17] including, for example, the random tempering [3,13]. The main difference between the SVM and other random optimization methods such as the random tempering is that the SVM employs the step-by-step procedure to build up a basis set, optimizing the nonlinear parameters of the basis states with respect to each other. The advantage of using the SVM here is that it seems to be quite suitable to find the optimal u vector.

The results for the positronium negative ion are compared to other calculations [22–27] in Table II. The energy obtained at the dimension \mathcal{K} is also shown. The trial function of case (i) does not produce good result, which is not surprising because the interparticle correlation is poorly represented in this case. The result of case (ii) shows a significant improvement over the case (i), confirming the importance of the polynomial part of type (4). The energy and the root mean square radius in this case are slightly better than our previous calculation [1]. This improvement is due to the refinement in the optimization of the nonlinear parameters, which were not employed before. A full correlated Gaussian basis of case (iii), though no polynomial part is employed, gives even better results which are comparable to the results obtained in the similar basis dimension by using the generalized Hylleraas-type wave functions [22,23]. Compared to the correlation-function hyperspherical harmonic (CFHH) method [25], our correlated Gaussian basis seems to give a better solution. The table also lists the calculated average distances between the two electrons and between the positron and an electron. They are in reasonable agreement with the most precise values obtained by using the correlated exponential (CE) functions [26] or the Hylleraas-type functions [27].

Table III lists the results for the lowest $L = 0-3$ states of the $t\bar{t}\mu$ molecule. This system is analogous to the negative positronium ion though the mass ratio of the constituent particles is considerably different. The results with the cases of (ii) and (iii) are shown and the quality

of them is similar to what is mentioned in the case of the negative positronium ion. Our calculation for the S and P states reproduces the first seven digits of Ref. [13] which uses the correlated Slater-type geminals or interparticle CE functions. For the D state our result is in good agreement with the extensive calculation of [14] using $\mathcal{K} = 2250$ basis functions similar to [13]. Both of them employ the bipolar harmonics of the stretched coupling to describe the rotational motion. The calculation of case (iii) uses $K_{\max} = 0$ so that the basis function in this case also employs only the stretched coupling. The fact that we have got rather accurate results in a small basis suggests that the usage of Eq. (6), particularly its angular part is very useful. We confirm that the F state is bound, in agreement with the other calculation [11], but have found no bound G state.

We next show in Table IV the results of calculation for the $dt\mu$ molecule. The basis functions of case (iii) again give better energies than those of case (ii). In fact they reproduce the first six digits of the most precise variational calculations [8,13,14] for $L = 0 - 2$ states. The Gaussian basis similar to case (ii) is employed in the GBCRC calculation of [8], where the angular part is, however, represented by the successive coupling of type (3). The fact that the D state energy of our calculation with $\mathcal{K} = 200$ becomes slightly lower than that of the GBCRC calculation with $\mathcal{K} = 1566$ confirms that a careful optimization of the nonlinear parameters is very important and moreover that the angular function of Eq. (4) is really useful. In Ref. [13] the optimized energy at smaller \mathcal{K} values is given for the S and P states. Our energies are slightly lower than theirs at the same dimension, which indicates the effectiveness of the basis optimization of the SVM.

Finally we present in Table V the energies of the helium atom which are obtained with cases (ii) and (iii). We used the finite mass of the α -particle, $m_\alpha = 7294.2618241m_e$. The basis functions of case (iii) give lower energies than those of (ii) for the S and P states but produce considerably higher energies for the states with higher L values. This suggests that the explicit introduction of the non-stretched coupling is more favorable to describe in our formulation the rotational motion of highly asymmetric states. In the table the energies of the S and P states are compared to the result of Ref. [15] where the bound states of the atomic and mesomolecular systems were studied up to $L = 2$ by using the CE functions of the interparticle distances. The angular part is expressed by the bipolar harmonics. The agreement is fair. To include the comparison with the combined configuration interaction Hylleraas method calculation [16], we repeated the calculation for the D and F states assuming the infinite mass for the α -particle. We see that our basis functions reproduce the energies of both states up to the first six-seven digits. The advantage of our method is that no special care is needed to treat states with high angular momenta.

IV. SUMMARY

We have presented a formulation for the correlated Gaussian basis which can describe the orbital motion with an arbitrary angular momentum. Instead of the well-known successive couplings of the spherical harmonics to the total orbital angular momentum the angular part of the basis functions in this formulation is uniquely represented by a single spherical harmonic of a global vector which is a linear combination of the relative coordinates. We have shown that this type of the correlated Gaussians is simply derived from the generating

function which is invariant with respect to the transformation of the relative coordinates. This property makes it much simpler to calculate the matrix elements and in fact the formulas for the matrix elements have been derived in a compact form for a general system of N -particles interacting with the central forces. They can be applied universally to diverse systems independently of the number of particles and of the total angular momentum. The extension to include the noncentral forces is straightforward. It should be noted that the present formulation for the angular part can be applied to other orbital functions as well as the correlated Gaussian.

The formulation has been applied to obtain the bound states of various Coulomb three-body systems which cover a wide range of mass ratio, namely, $e^-e^-e^+$, $tt\mu$, $td\mu$, and αe^-e^- . The basis functions have been set up stepwise in a trial and error procedure using the stochastic variational method. The coefficients defining the global vector can be varied continuously to minimize the energy. The nonlinear parameters of the correlated Gaussians are parametrized by three different options. One of the options is to include only the so-called rearrangement channels with the angular functions which describe the non-stretched coupling. This model has already given fairly good results. Compared to the restricted case in which only the stretched coupling is included, this option presents much better results. The other option is to use the full matrices to include the correlation between the particles. This model, even without use of the polynomial part, has been better than the former model in most cases but the high L states of the helium atom and, with the basis size of 200, reproduced the first six–seven digits of the total binding energies of almost all the systems mentioned above. We have tested the bound states up to $L = 4$ and found that no difficulty arises from the treatment of high angular momentum states in our formulation. We have confirmed that the correlated Gaussian of type (6) works very nicely as a basis function for bound-state solution for diverse systems. Although we suggested the method to treat the unnatural parity case, a more unified representation for both natural and unnatural parity cases should be developed.

Finally we summarize some merits of our method in the following.

- (i) No partial wave expansion is needed, and thus no problems in angular momentum coupling arise.
- (ii) Universality of the scheme. One needs to introduce no change, for example, when treating a larger system of N -particles or describing states with high angular momentum. There is no center-of-mass motion problem.
- (iii) Invariance with respect to the coordinate transformation. The form of basis states is kept invariant under the transformation. It is easy to construct the symmetry-adapted basis states.
- (iv) Fully analytical calculational scheme. The matrix elements are evaluated as simply as those for $L = 0$. The dependence of the matrix elements on the nonlinear parameters has simple structure.

This work was supported by Grants-in-Aid for Scientific Research (No. 05243102 and No. 06640381) and for International Scientific Research (Joint Research) (No. 08044065) of

the Ministry of Education, Science and Culture (Japan) and by OTKA grant No. T17298 (Hungary). The authors are grateful for the use of RIKEN's computer facility which made possible most of the calculations. Thanks are also due to the support of both Japan Society for the Promotion of Science and Hungarian Academy of Sciences.

APPENDIX

We prove by induction that the vector-coupled function of two solid spherical harmonics

$$\left[\mathcal{Y}_{l_1}(\mathbf{x}_1)\mathcal{Y}_{l_2}(\mathbf{x}_2)\right]_{LM} \quad \text{with} \quad (-1)^{l_1+l_2} = (-1)^L \quad (34)$$

can be expressed in terms of a linear combination of terms

$$|\mathbf{x}_1|^{2p_1}|\mathbf{x}_2|^{2p_2}|\mathbf{v}|^{2q+L}Y_{LM}(\hat{\mathbf{v}}), \quad (35)$$

where the degree of the function is given by $2p_1 + 2p_2 + 2q + L = l_1 + l_2$, and the vector \mathbf{v} of each term is given by $\mathbf{v} = u_1\mathbf{x}_1 + u_2\mathbf{x}_2$ with appropriate coefficients u_1 and u_2 .

First we prove that the statement is true for a special case of $l_1 + l_2 = L$, namely for the lowest order terms for a given L . As Eq. (5) shows, $|\mathbf{v}|^LY_{LM}(\hat{\mathbf{v}})$ consists of $L + 1$ terms of $\left[\mathcal{Y}_l(\mathbf{x}_1)\mathcal{Y}_{L-l}(\mathbf{x}_2)\right]_{LM}$ ($l = 0, 1, \dots, L$), each multiplied by $u_1^l u_2^{L-l}$. By using $L + 1$ mutually different u_1 values, $(u_1^{(1)}, u_1^{(2)}, \dots, u_1^{(L+1)})$, in Eq. (5) and keeping u_2 an arbitrary constant, it is possible to pick up a particular term $\left[\mathcal{Y}_l(\mathbf{x}_1)\mathcal{Y}_{L-l}(\mathbf{x}_2)\right]_{LM}$ through a linear combination of $\sum_{\alpha=1}^{L+1} c_\alpha |\mathbf{v}_\alpha|^LY_{LM}(\hat{\mathbf{v}}_\alpha)$ with $\mathbf{v}_\alpha = u_1^{(\alpha)}\mathbf{x}_1 + u_2\mathbf{x}_2$, where c_α should satisfy the following equation

$$\sum_{\alpha=1}^{L+1} (u_1^{(\alpha)})^m c_\alpha = \delta_{ml}, \quad \text{for } m = 0, 1, \dots, L. \quad (36)$$

The solution of the above linear equation for c_α is given by Vandermonde's determinant. Thus our assertion is proved.

Next we assume that the statement holds for all the cases of $l_1 + l_2 \leq 2(K - 1) + L$. We note that all the terms of $\left[\mathcal{Y}_{K+l}(\mathbf{x}_1)\mathcal{Y}_{K+L-l}(\mathbf{x}_2)\right]_{LM}$ ($l = 0, 1, \dots, L$) with degree $2K + L$ appear in the expansion of Eq. (5) together with the respective coefficients $u_1^{K+l}u_2^{K+L-l}$. The rest of the terms in the expansion can, by assumption, be expressed in the form of Eq. (35) because the vector-coupled part of each term has smaller degree than $2K + L$. Using $L + 1$ different u_1 values similarly to the above case of Eq. (36) enables us to express each of the terms, $\left[\mathcal{Y}_{K+l}(\mathbf{x}_1)\mathcal{Y}_{K+L-l}(\mathbf{x}_2)\right]_{LM}$, in terms of a linear combination of the functions of Eq. (35). This completes the proof.

REFERENCES

- [1] K. Varga and Y. Suzuki, Phys. Rev. **C52**, 2885 (1995); Phys. Rev. **A53**, 1907 (1996).
- [2] S. F. Boys, Proc. R. Soc. London Ser. **A258**, 402 (1960); K. Singer, *ibid.* **A258**, 412 (1960).
- [3] S. A. Alexander, H. J. Monkhorst, and K. Szalewicz, J. Chem. Phys. **85**, 5821 (1986).
- [4] P. M. Kozłowski and L. Adamowicz, J. Chem. Phys. **95**, 6681 (1991).
- [5] D. B. Kinghorn and R. D. Poshusta, Phys. Rev. **A47**, 3671 (1993).
- [6] W. Cencek and J. Rychlewski, J. Chem. Phys. **98**, 1252 (1993).
- [7] A. M. Frolov and V. H. Smith, Jr., Phys. Rev. **A53**, 3853 (1996) and references therein.
- [8] M. Kamimura, Phys. Rev. **A38**, 621 (1988).
- [9] H. Kameyama, M. Kamimura, and Y. Fukushima, Phys. Rev. **C40**, 974 (1989).
- [10] K. Varga, Y. Ohbayasi, and Y. Suzuki, to be published in Phys. Lett. B.
- [11] S. I. Vinitskiĭ, V. S. Melezhik, L. I. Ponomarev, I. V. Puzynin, T. P. Puzynina, L. N. Somov, and N. F. Truskova, Sov. Phys. JETP **52**, 353 (1980).
- [12] A. K. Bhatia and R. J. Drachman, Phys. Rev. **A30**, 2138 (1984).
- [13] S. A. Alexander and H. J. Monkhorst, Phys. Rev. **A38**, 26 (1988).
- [14] A. M. Frolov, V. H. Smith, Jr., and D. M. Bishop, Phys. Rev. **A49**, 1686 (1994); *ibid.* **A51**, 3636 (1995).
- [15] A. M. Frolov, Sov. Phys. JETP **65**, 1100 (1987).
- [16] J. S. Sims and W. C. Martin, Phys. Rev. **A37**, 2259 (1988).
- [17] See, for example, R. Bukowski, B. Jeziorski, S. Rybak, and K. Szalewicz, J. Chem. Phys. **102**, 888 (1995).
- [18] K. Arai, Y. Suzuki, and K. Varga, Phys. Rev. **C51**, 2488 (1995); K. Varga, Y. Suzuki, and I. Tanihata, *ibid.* **C52**, 3013 (1995).
- [19] D. P. Chong and D. M. Schrader, Mol. Phys. **16**, 137 (1969).
- [20] V. I. Kukulin and V. M. Krasnopol'sky, J. Phys. **G3**, 795 (1977).
- [21] K. Varga, Y. Suzuki, and R. G. Lovas, Nucl. Phys. **A571**, 447 (1994).
- [22] Y. K. Ho, J. Phys. **B16**, 1503 (1983).
- [23] A. K. Bhatia and R. J. Drachman, Phys. Rev. **A28**, 2523 (1983).
- [24] A. Yeremin, A. M. Frolov, and E. B. Kutukova, Few-Body Systems **4**, 111 (1988).
- [25] R. Krivec, M. I. Haftel, and V. B. Mandelzweig, Phys. Rev. **A47**, 911 (1993).
- [26] A. M. Frolov, J. Phys. **B26**, 1031 (1993).
- [27] Y. K. Ho, Phys. Rev. **A48**, 4780 (1993).

TABLES

TABLE I. Possible sets of partial waves contained in a single spherical harmonic with low L and K values for a three-body system. See Eq. (5). Listed below are only the cases of $2k_1 + l_1 \leq 2k_2 + l_2$.

L	K	k_1	l_1	k_2	l_2
0	0	0	0	0	0
		0	0	1	0
	1	0	1	0	1
		0	0	2	0
		0	1	1	1
		0	2	0	2
		1	0	1	0
1	0	0	0	0	1
	1	0	0	1	1
		0	1	0	2
		0	1	1	0
	2	0	0	2	1
		0	1	1	2
		0	1	2	0
		0	2	0	3
		0	2	1	1
		1	0	1	1
		1	0	1	1
2	0	0	0	0	2
		0	1	0	1
	1	0	0	1	2
		0	1	0	3
		0	1	1	1
		0	2	0	2
		0	2	1	0
		1	0	0	2
		1	0	0	2
	2	0	0	2	2
		0	1	1	3
		0	1	2	1
		0	2	0	4
		0	2	1	2
		0	2	2	0
		1	0	1	2
		0	3	0	3
		0	3	1	1
		1	1	0	3
		1	1	1	1
3	0	0	0	0	3
		0	1	0	2
	1	0	0	1	3
		0	1	0	4

	0	1	1	2
	0	2	0	3
	0	2	1	1
	1	0	0	3
2	0	0	2	3
	0	1	1	4
	0	1	2	2
	0	2	0	5
	0	2	1	3
	0	2	2	1
	1	0	1	3
	0	3	0	4
	0	3	1	2
	0	3	2	0
	1	1	0	4
	1	1	1	2

TABLE II. The total binding energy and the distance of the $e^-e^-e^+$ system. \mathcal{K} is the number of basis functions used. See text for the cases (i), (ii), and (iii) of basis functions. Atomic units are used.

basis function	\mathcal{K}	energy	radius	$< r^2 >^{1/2}$		$< r >$	
				e^-e^+	e^-e^-	e^-e^+	e^-e^-
(i)	50	0.26186974					
	100	0.26188326	4.596	6.968	9.644	5.494	8.539
	150	0.26188401					
	200	0.26188445	4.597	6.96882	9.64479	5.49475	8.54000
(ii)	50	0.26199779					
	100	0.26200455	4.594	6.958	9.652	5.489	8.548
	150	0.26200489					
	200	0.26200494	4.595	6.95835	9.65285	5.48963	8.54856
(iii)	50	0.26199953					
	100	0.26200465	4.594	6.958	9.652	5.489	8.548
	150	0.26200491					
	200	0.26200504	4.595	6.95812	9.65254	5.48957	8.54846
<hr/>							
Hylleraas [22]	125	0.262004895		6.957	9.650	5.4891	8.5476
Hylleraas [23]	220	0.2620050565					
CFHH [25]	225	0.262004673		6.956	9.650	5.48881	8.54699
CE [26]	800	0.2620050702319		6.95837	9.65291	5.4896332525	8.5485806553
Hylleraas [27]	744	0.2620050702328		6.95837	9.65291	5.489633252	8.548580655

TABLE III. The total binding energies and the rms distances of the lowest S , P , D , and F states of the $tt\mu$ system. The mass set used is $m_t = 5496.918m_e$, and $m_\mu = 206.7686m_e$. Atomic units are used.

L	basis function	\mathcal{K}	energy	$\langle r^2 \rangle^{1/2} \times 10^3$		
				radius	$t\mu$	tt
S	(ii)	200	112.97253	7.444	11.15	13.39
	(iii)	200	112.97300	7.444	11.15	13.39
	CE [13]	500	112.9730179			
P	(ii)	200	110.26189	7.933	11.82	14.46
	(iii)	200	110.26210	7.933	11.82	14.46
	CE [13]	500	110.2621165			
D	(ii)	200	105.98288	8.919	13.18	16.59
	(iii)	200	105.98301	8.919	13.18	16.59
	(iii) ^a	200	105.98292	8.919	13.18	16.59
	CE [14] ^a	2250	105.982930			
F	(ii)	200	101.43093	10.71	15.67	20.39
	(iii)	200	101.43105	10.71	15.67	20.38
	(iii) ^b	200	101.43131	10.71	15.67	20.39
	Adiabatic [11] ^b		101.43			

^a $m_t = 5496.92158m_e$, $m_\mu = 206.768262m_e$, $2R_\infty = 27.2113961\text{eV}$.

^b $m_t = 5496.918m_e$, $m_\mu = 206.769m_e$, $R_\infty = 13.6058\text{eV}$.

TABLE IV. The total binding energies and the rms distances of the lowest S , P , and D states of the $td\mu$ system. The mass set used is $m_t = 5496.918m_e$, $m_d = 3670.481m_e$, and $m_\mu = 206.7686m_e$. Atomic units are used.

L	basis function	\mathcal{K}	energy	$\langle r^2 \rangle^{1/2} \times 10^3$			
				radius	$d\mu$	$t\mu$	td
S	(ii)	100	111.36357	7.774	11.73	11.24	13.92
		200	111.36398	7.774	11.73	11.24	13.92
	(iii)	100	111.36363	7.774	11.73	11.24	13.92
		200	111.36444	7.774	11.73	11.24	13.92
	GBCRC [8]	1442	111.364507				
	CE [13]	1400	111.364511474				
P	(ii)	100	108.17803	8.417	12.68	12.03	15.31
		200	108.17914	8.417	12.68	12.03	15.31
	(iii)	100	108.17820	8.416	12.68	12.03	15.31
		200	108.17940	8.417	12.68	12.03	15.31
	CE [13]	1800	108.1795424				
	(iii) ^a	200	108.17923	8.417	12.68	12.03	15.31
	GBCRC [8] ^a	2662	108.179385				
D	(ii)	100	103.40632	9.766	14.81	13.61	18.19
		200	103.40824	9.769	14.81	13.61	18.19
	(iii)	100	103.40733	9.766	14.81	13.61	18.19
		200	103.40849	9.769	14.81	13.61	18.19
	GBCRC [8]	1566	103.408481				

^a $m_t = 5496.92158m_e$, $m_d = 3670.483014m_e$, $m_\mu = 206.768262m_e$, $R_\infty = 13.6056981\text{eV}$.

TABLE V. The total binding energies and the rms distances of the lowest S , P , D , F , and G states of the helium atom (αe^-e^-). The correlated Gaussians of cases (ii) and (iii) are used for basis functions. The α -particle mass is $m_\alpha = 7294.2618241m_e$. Atomic units are used.

L	basis function	\mathcal{K}	energy	$< r^2 >^{1/2}$		
				radius	$e^-\alpha$	e^-e^-
1^1S	(ii)	200	2.9033033	0.8920	1.093	1.587
	(iii)	200	2.9033041	0.8920	1.093	1.587
	CE [15]	300	2.903304555			
2^3S	(ii)	200	2.1749299	2.765	3.386	4.801
	(iii)	200	2.1749299	2.765	3.386	4.801
	CE [15]	over 350	2.174930189			
2^1P	(ii)	200	2.1235432	3.242	3.971	5.622
	(iii)	200	2.1235446	3.242	3.971	5.622
	CE [15]	over 350	2.123545653			
2^3P	(ii)	200	2.1328785	2.968	3.635	5.162
	(iii)	200	2.1328798	2.967	3.635	5.162
	CE [15]	over 350	2.132880641			
3^1D	(ii)	200	2.0553385	6.489	7.949	11.244
	(iii)	200	2.0553377	6.489	7.948	11.243
	(ii) ^a	200	2.0556201	6.488	7.948	11.242
	(iii) ^a	200	2.0556195	6.488	7.947	11.242
	Hylleraas [16] ^a	438	2.05562073279			
3^3D	(ii)	200	2.0553538	6.486	7.945	11.239
	(iii)	200	2.0553531	6.486	7.945	11.238
	(ii) ^a	200	2.0556355	6.485	7.944	11.237
	(iii) ^a	200	2.0556349	6.485	7.944	11.237
	Hylleraas [16] ^a	393	2.05563630941			
4^1F	(ii)	200	2.03097661	10.963	13.429	18.992
	(iii)	200	2.03097596	10.962	13.427	18.990
	(ii) ^a	200	2.03125504	10.962	13.427	18.989
	(iii) ^a	200	2.03125314	10.960	13.425	18.987
	Hylleraas [16] ^a	438	2.03125514434			
4^3F	(ii)	200	2.03097664	10.963	13.429	18.992

	(iii)	200	2.03097598	10.962	13.427	18.990
	(ii) ^a	200	2.03125506	10.961	13.427	18.989
	(iii) ^a	200	2.03125317	10.960	13.425	18.987
	Hylleraas [16] ^a	438	2.03125516836			
5 ¹ G	(ii)	200	2.0197237802	16.589	20.321	28.738
	(iii)	200	2.0197114443	16.553	20.276	28.675
5 ³ G	(ii)	200	2.0197237803	16.589	20.321	28.738
	(iii)	200	2.0197114445	16.553	20.276	28.675

^a The mass of the α -particle is assumed to be infinite.